AMENDMENTS TO THE CLAIMS

This listing of claims will replace all prior versions of claims in the application.

1. (Currently amended) A p~~P~~rocess for the discovery and preparation of new compounds, characterised by

(1) selection of M different starting materials ~~suitable~~ for multicomponent reactions (MCRs),

(2) chemical reaction of each starting material with every possible combination of from 2 to M-1 other starting materials selected according to (1) to provide products,

(3) analysis of the products for one or more biological, pharmacological, or physicochemical criterion,

(4) evaluation of ~~the~~one or more products based on one or more biological, pharmacological, or physicochemical criterion and selection of at least one product based on one or more biological, pharmacological, or physicochemical criterion,

(5) determination of the starting materials that have led to the product(s) selected in (4), and

(6) provision of at least one variant of at least one of the starting materials that have been determined in (5),

(7) reaction of the starting materials provided in (6) with the remaining starting materials determined in (5) or variants thereof in the context of an MCR,

(8) repetition of steps (4) to (7) until at least one new product having the desired property or properties is found, and

(9) optionally isolation and physicochemical characterisation of the product.

2. (Currently amended) The p~~P~~rocess according to claim 1, characterised in that M=<40.

3. (Currently amended) The p~~P~~rocess according to claim 1, characterised in that in (1) and/or in (6) reaction conditions ~~suitable~~ for MCRs are also selected.

4. (Cancelled)

5. (Cancelled)

6. (Currently amended) The pProcess according to claim 1, characterised in that in (4) all products are evaluated.

7. (Currently amended) The pProcess according to claim 1, characterised in that in (4) the reaction conditions for preparing the products are also evaluated.

8. (Currently amended) The pProcess according to claim 1, characterised in that the reaction according to (7) of the starting materials provided in (6) is ~~if appropriate~~ carried out with the remaining starting materials determined in (5) with the exception of the starting material(s) of which variants were provided in (6).

9. (Currently amended) The pProcess according to claim 1, characterised in that for each reaction according to (7) only one molecule is selected per starting material type.

10. (Currently amended) The pProcess according to claim 1, wherein each of the starting materials has~~ve~~ at least one functional group that is ~~s customary in organic chemistry, such as~~ -NC, -CO-, -CS-, -CN, -OCN, -NCO, -NO, $-NO_2$, $-ONO_2$, -CHO, -COOR, -COSR, -CSSR, -COCOOR, -SCN, -NCS, -halo, $-N_3$, -NNNR, -OR, -SR, -OCOOR, -SCOOR, -NRCOOR', -OCSOR, -SCSOR, -NRCSOR', -OCSSR, -SCSSR, -NRCSSR', -OCONR'R, -SCONR'R, -NRCONR'R'', -NRR'', -NRR'NR''R''', -CNNRR', -CNNRR'HX, -NRCONR'R'', -NRCSNR'R'', -RCOCR'R'', -RCSCR'R'', -COCRR'halo, -RCNR 'CR'', wherein R, R' and R'' are H or alkyl, aryl, aralkyl, hetaryl or hetarylalkyl.

11. (Currently amended) The pProcess according to claim 10, wherein the functional groups are epoxy groups or carbenes or the unsaturated vinylogous variants alkene, alkyne, aryl groups or corresponding mono-, di-, tri-, tetra-, penta- or hexa-carbonyl variants of those groups.

12. (Currently amended) The pProcess according to claim 10 or 11, wherein two, three, four or more functional groups are present simultaneously in one or more starting materials in suitable combination.

13. (Currently amended) The pProcess according to claim 10, wherein the starting materials are starting materials especially suitable for multicomponent reactions, such as alpha-halokctones, esters, carboxylic acids, thiocarboxylic acids, aldehydes, amines, ketones, isonitriles, nitriles, alpha-keto acids, alpha-keto esters, and derivatives and alpha-beta unsaturated variants thereof, and also combinations thereof.

14. (Currently amended) The pProcess according to claim 1[[4]], wherein the starting materials have corresponding mono-, di-, tri-, tetra-, penta- or hexa-carbonyl variants of the functional groups.

15. (Currently amended) The pProcess according to claim 1, wherein some of the functional groups of the starting materials are protected~~provided~~ with protecting groups customary in organic chemistry.

16. (Currently amended) The pProcess according to claim 1, wherein the selected starting materials are encoded in a form accessible to an algorithm, the selected starting materials being assigned, either randomly or systematically, unambiguous binary, decimal or alphanumeric codings.

17. (Currently amended) The pProcess according to claim 1, wherein a starting material type of a specific chemical class is assigned a characteristic coding for that chemical class.

18. (Currently amended) The pProcess according to claim 1, wherein in the first cycle of the process only those starting materials which belong to different chemical classes are selected.

19. (Currently amended) The p~~P~~rocess according to claim 1, wherein the starting materials are selected in accordance with an algorithm.

20. (Currently amended) The p~~P~~rocess according to claim 1, wherein multicomponent combinations MCC(K) selected in accordance with an algorithm of different selected starting materials are reacted simultaneously or in a sequential order under conditions customary in organic chemistry.

21. (Currently amended) The p~~P~~rocess according to claim 1, wherein each selected combination of starting materials is reacted in a physically separate, optionally encoded reaction vessel.

22. (Currently amended) The p~~P~~rocess according to claim 1, wherein at least some of the resulting reaction products are, in a subsequent step, chemically modified, worked-up or prepared for step (3) ~~in a suitable manner~~.

23. (Currently amended) The p~~P~~rocess according to claim 1, wherein additional auxiliaries or catalysts that are~~, such as, for example,~~ Lewis acids, ~~such as boron trifluoride etherate, zinc chloride, ytterbium triflate, iron chloride, other~~ acids, ~~such as, for example, hydrochloric acid, paratoluenesulfonic acid, acetic acid, or~~ bases, ~~such as, for example, potassium carbonate, triethylamine, caesium carbonate,~~ or water-removing agents~~, such as molecular sieves or orthoesters,~~ are used.

24. (Currently amended) The p~~P~~rocess according to claim 22 or 23, wherein the chemical modification is the removal of chemical protecting groups~~, for example~~ by ~~trifluoroacetic~~ acid, or the hydrogenation of the products ~~by means of hydrogen, optionally with the addition of a hydrogenation catalyst, such as palladium on carbon, platinum oxide, palladium acetate~~, or by oxidation of the products ~~with oxygen or some other oxidising agent, such as, for example, bromine,~~

~~hydrogen peroxide, tert-butyl peroxide or a suitable metal salt, such as cobalt chloride, or a suitable metal complex, such as, for example, iron hexacyanoferrate or chromium tetraphenylporphyrinate~~, or by irradiation with light of wavelength 200-600 nm, or the reaction products are treated with at least one enzyme~~, such as, for example, oxidoreductases, ligases, peptidases, lipases or isomerases~~.

25. (Currently amended) The p~~P~~rocess according to claim 22, wherein the working-up of the products is carried out in a manner known per se by chromatography~~, for example over silica gel or RP-18 silica gel~~, or solid phase extraction or the removal of unreacted starting materials by binding to a suitable solid carrier, such as, for example, ion exchanger resins or chemically modified solid phase resins, or by selective binding of the products to a suitable solid carrier.

26. (Currently amended) The p~~P~~rocess according to claim 20 or 23, wherein the reaction conditions and auxiliaries used or catalysts are assigned, either randomly or systematically, unambiguous binary, decimal or alphanumeric codings.

27. (Currently amended) The p~~P~~rocess according to claim 21, wherein the allocation of the various encoded combinations to the reaction vessels is encoded, either randomly or systemically, in binary, decimal or alphanumeric form.

28. (Currently amended) The p~~P~~rocess according to claim 22 or 25, wherein the working-up of the products is assigned, either randomly or systematically, binary, decimal or alphanumeric codings.

29. (Currently amended) The p~~P~~rocess according to claim 1, wherein both the starting materials, reaction conditions, modifications, working-up procedures or procedures in preparation for testing that are used and the reaction vessels are encoded.

30. (Currently amended) The p~~P~~rocess according to claim 1, where the MCR is a Passerini or Ugi multicomponent reaction with up to 20 components~~, preferably with 3, 4, 5, 6, 7, 8, 9, 10, 11 or 12 components~~.

31. (Currently amended) The p~~P~~rocess according to claim 1, wherein the products are investigated in a biological and/or pharmacological test for their pharmacological or biological activity, effectiveness, side effects and/or selectivity and/or in a further test procedure for their physico-chemical properties.

32. (Currently amended) The p~~P~~rocess according to claim 31, wherein the dependency of the measurement results upon the concentration of the starting materials used in process step two is ascertained, the concentration lying especially in a range of from 0.5 to 0.000001 mol/l.

33. (Currently amended) The p~~P~~rocess according to claim 32, wherein the concentration lies in a range of from 100 to 0.01 mol/l.

34. (Currently amended) The p~~P~~rocess according to any one of claims 31 to 33, wherein the test for ascertaining the biological or pharmacological activity, effectiveness, side effects or selectivity is carried out with isolated proteins, receptors, enzymes, or mixtures thereof, cells, cell lysates, complex cell systems, with organs or parts thereof or a plurality of organs or with whole organisms or membranes and ~~as appropriate~~ optionally using adjuvants, substrates or detection aids necessary for the test.

35. (Currently amended) The p~~P~~rocess according to any one of claims 31 to 33, wherein the test procedures for the physico-chemical properties of the products include the measurement of the lipophilicity by means of the octanol-water distribution coefficient, the solubility in water, the non-specific protein binding to, for example, bovine serum albumin, the binding to the proteins of human serum plasma and/or the chemical stability in Krebs buffer.

36. (Currently amended) The p~~P~~rocess according to claim 1, wherein the test results obtained are related to the codings of the individual reaction products.

37. (Currently amended) The p~~P~~rocess according to claim 36, wherein the test results are stored in a form accessible to an algorithm~~, for example in a computer data file or a computer data bank~~.

38. (Currently amended) The p~~P~~rocess according to claim 1, wherein the list of the codings and the associated test results fulfil all the prerequisites necessary for further optimisation.

39. (Currently amended) The p~~P~~rocess according to claim 1, wherein the codings of the products prepared and tested are evaluated, the genomes either being sorted by ranking or divided into various evaluation categories, in accordance with a predetermined target function.

40. (Currently amended) The p~~P~~rocess according to claim 39, wherein the target function may be any desired function construed from the combination of desired properties of the target compounds.

41. (Currently amended) The p~~P~~rocess according to claim 38 ~~or 40~~, wherein the evaluation criterion for the sorting or categorisation of the genomes is derived from the extent to which the individual products fulfil the target function.

42. (Currently amended) The p~~P~~rocess according to any one of claims 39 to 41 or 70, wherein the biological activity, the physico-chemical properties and optionally further biologically relevant test results form the target function.

43. (Currently amended) The p~~P~~rocess according to any one of claims 39 to 41 or 70~~2~~, wherein the concentration dependency of the test results is included in the target function.

44. (Currently amended) The pProcess according to claim 40, wherein the properties are included in the target function with different and concentration-dependent weighting, the target function ~~especially~~ being a linear combination or polynome of those properties with "fuzzy" logic weightings.

45. (Currently amended) The pProcess according to claims 40, wherein the "fuzzy" logic weightings of individual properties are dependent upon the extent to which other properties are fulfilled and upon the number of cycles already completed.

46. (Currently amended) The pProcess according to claim 1, wherein the evaluated codings of the individual products are utilised to find a new set of optionally encoded starting materials, reaction conditions, modification and working-up procedures using a combinatorial optimisation procedure, ~~such as, for example, a genetic algorithm or a pattern recognition process, a neuronal network or a combination of a genetic algorithm with a neuronal network, and~~ to carry out corresponding MCRs.

47. (Currently amended) The pProcess according to claim 1, wherein a reaction that has already been performed is not repeated.

48. (Currently amended) The pProcess according to claim 46 or 47, wherein the codings from the preceding cycle that are evaluated as being the ~~best~~ highest ranked are used in the next cycle.

49. (Currently amended) The pProcess according to claims 11, wherein preferably a genetic algorithm or a pattern recognition process, such as a neuronal network or a combination of a genetic algorithm with a neuronal network, implicitly or explicitly correlates the occurrence of desired properties with the constituents of the coding of the corresponding product of the preceding cycles.

50. (Currently amended) The pProcess according to claim 49, wherein those constituents of the coding of the tested products which with greater probability correlate explicitly or implicitly with the desired properties are used with greater probability for the generation of new codings.

51. (Currently amended) The pProcess according to claim 49, wherein codings that have not received a good rating are not used for the generation of new codings.

52. (Currently amended) The pProcess according to claim 49 or 50, wherein individual constituents of the new codings are selected from the number of possible codings by means of a random generator.

53. (Currently amended) The pProcess according to claim 49[[,] or 50 ~~or 52~~ wherein individual constituents of the new codings are removed from or added to the genome by means of a random generator.

54. (Currently amended) The pProcess according to claim 52 ~~or 53~~, wherein the assignment of probability to a random selection of such a building block depends upon the type of that building block.

55. (Currently amended) The pProcess according to claim 52, ~~53 or 54,~~ wherein the codings are divided randomly into one or more groups, so-called populations, the codings of a group especially being used only for the generation of new codings of a new group of genomes, each of those populations thus creating a new population.

56. (Currently amended) The pProcess according to claim 55, wherein after any desired number of cycles all populations of genomes are divided up into a new number of populations having the same number or a different number of genomes.

57. (Currently amended) The pProcess according to claim 56, wherein that new division is carried out when in a population a product has ~~especially~~ desirable properties.

58. (Currently amended) The pProcess according to claim 1, wherein up to 30 cycles are required to find a product having ~~especially~~ desirable properties.

59. (Currently amended) The pProcess according to claim 58, wherein the probability of discovering such a product is estimated after as few as 2 to 6 cycles by means of the difference between the average extent to which the products of a population from a cycle x fulfil the target criteria and the average extent to which the products of a population from a later cycle x+i fulfil the target criteria, where i is a whole natural number.

60. (Currently amended) The pProcess according to claim 59, wherein that difference can be used to select a new number of starting materials, reaction conditions, modifications or working-up procedures and to begin the iterative process afresh.

61. (Currently amended) The pProcess according to claim 60, wherein the iterative process is begun afresh when the difference is small.

62. (Currently amended) The pProcess according to claim 1, wherein the chemical compounds contained in the reaction product that has exhibited the desired properties in the tests are purified and the structure thereof is determined.

63. (Currently amended) The pProcess according to claim 1, wherein the analysis of the products is an investigation into whether the product has therapeutic properties.

64. (New) The process according to claim 23, wherein the additional auxiliaries or catalysts are boron trifluoride etherate, zinc chloride, ytterbium triflate,

iron chloride, hydrochloric acid, paratoluenesulfonic acid, acetic acid, potassium carbonate, triethylamine, caesium carbonate, or molecular sieves or orthoesters.

65. (New) The process according to claim 24, wherein the chemical modification is the removal of chemical protecting groups by acid, or the hydrogenation optionally with the addition of a hydrogenation catalyst, or by oxidation with oxygen or some other oxidising agent, or by irradiation with light of wavelength 200-600 nm, or treatment with at least one enzyme.

66. (New) The process according to claim 65, wherein the chemical modification is the removal of chemical protecting groups by trifluoroacetic acid, or the hydrogenation optionally with the addition of a hydrogenation catalyst that is palladium on carbon, platinum oxide, palladium acetate, or by oxidation with oxygen or some other oxidising agent, that is bromine, hydrogen peroxide, tert-butyl peroxide or a suitable metal salt, that is cobalt chloride, or metal complex, that is iron hexacyanoferrate or chromium tetraphenylporphyrinate, or by irradiation with light of wavelength 200-600 nm, or treatment with at least one enzyme that is a oxidoreductase, ligase, peptidase, lipase or isomerase.

67. (New) The process of claim 30, wherein the up to 20 components, is 3, 4, 5, 6, 7, 8, 9, 10, 11 or 12 components.

68. (New) The process of claim 37, wherein the test results are stored in a form accessible to an algorithm in a computer data file or a computer data bank.

69. (New) The process of claim 46, wherein the combinatorial optimisation procedure is a genetic algorithm or a pattern recognition process, a neuronal network or a combination of a genetic algorithm with a neuronal network.

70. (New) The process according to claim 40, wherein the evaluation criterion for the sorting or categorisation of the genomes is derived from the extent to which the individual products fulfill the target function.

71. (New) The process according to any one of claims 39-41 or 70, wherein the biological activity, the physico-chemical properties and optionally further biologically relevant test results form the target function, and wherein the concentration dependency of the test results is included in the target function.

72. (New) The process according to claim 49 or 50, wherein individual constituents of the new codings are selected from the number of possible codings by means of a random generator, and wherein individual constituents of the new codings are removed from or added to the genome by means of a random generator.

73. (New) The process according to claim 49 or 50, wherein individual constituents of the new codings are removed from or added to the genome by means of a random generator, and the assignment of probability to a random selection of such a building block depends upon the type of that building block.

74. (New) The process according to claim 49 or 50, wherein individual constituents of the new codings are selected from the number of possible codings by means of a random generator, individual constituents of the new codings are removed from or added to the genome by means of a random generator, and the assignment of probability to a random selection of such a building block depends upon the type of that building block.

75. (New) The process according to claim 49 or 50, wherein individual constituents of the new codings are removed from or added to the genome by means of a random generator, and the codings are divided randomly into one or more groups, so-called populations, the codings of a group especially being used only for the generation of new codings of a new group of genomes, each of those populations thus creating a new population.

76. (New) The process according to claim 49 or 50, wherein individual constituents of the new codings are selected from the number of possible codings by

means of a random generator, individual constituents of the new codings are removed from or added to the genome by means of a random generator, and the codings are divided randomly into one or more groups, so-called populations, the codings of a group especially being used only for the generation of new codings of a new group of genomes, each of those populations thus creating a new population.

77. (New) The process according to claim 49 or 50, wherein individual constituents of the new codings are selected from the number of possible codings by means of a random generator, the assignment of probability to a random selection of such a building block depends upon the type of that building block, and the codings are divided randomly into one or more groups, so-called populations, the codings of a group especially being used only for the generation of new codings of a new group of genomes, each of those populations thus creating a new population.

78. (New) The process according to claim 49 or 50, wherein individual constituents of the new codings are selected from the number of possible codings by means of a random generator, individual constituents of the new codings are removed from or added to the genome by means of a random generator, the assignment of probability to a random selection of such a building block depends upon the type of that building block, and the codings are divided randomly into one or more groups, so-called populations, the codings of a group especially being used only for the generation of new codings of a new group of genomes, each of those populations thus creating a new population.

79. (New) The process according to claim 75, wherein after any desired number of cycles all populations of genomes are divided up into a new number of populations having the same number or a different number of genomes.

80. (New) The process according to claim 76, wherein after any desired number of cycles all populations of genomes are divided up into a new number of populations having the same number or a different number of genomes.

81. (New) The process according to claim 77, wherein after any desired number of cycles all populations of genomes are divided up into a new number of populations having the same number or a different number of genomes.

82. (New) The process according to claim 78, wherein after any desired number of cycles all populations of genomes are divided up into a new number of populations having the same number or a different number of genomes.

83. (New) The process according to claim 79, wherein that new division is carried out when in a population a product has desirable properties.

84. (New) The process according to claim 80, wherein that new division is carried out when in a population a product has desirable properties.

85. (New) The process according to claim 81, wherein that new division is carried out when in a population a product has desirable properties.

86. (New) The process according to claim 82, wherein that new division is carried out when in a population a product has desirable properties.